1,4-Ethanonaphtho(1,8-ef)-1,4-diazepine, 2,3-dihydro-

59950-41-3 | DTXSID40208664

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 642 L/kg

Global applicability domain: Outside

Local applicability domain index: 2.15e-01

Confidence level: 5.38e-01

Nearest Neighbors from the Training Set

Image not found

Methapyrilene
Measured: 741
Predicted: 682

Image not found

Hexazinone
Measured: 53.7
Predicted: 67.1

Image not found

Auramine
Measured: 2040
Predicted: 1020

Image not found

4,4'-Methylenebis(N,N-dimethylaniline)
Measured: 9120
Predicted: 3540

Image not found

Michler's ketone
Measured: 162
Predicted: 489